

# Quadrilateral quantum chain Hamiltonian cast in positive semidefinite form containing non-linear fermionic contributions

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*Abstract:* The transformation of a Hamiltonian (connected to a quantum mechanical many-body system) in positive semidefinite form represents an important procedure in a powerful tool used in deducing exact results for non-integrable systems. Motivated by this fact, we report in this paper the exact transformation of a Hubbard type of Hamiltonian (describing in the presented case an itinerant fermionic quadrilateral chain) in positive semidefinite form, in a such a way that the kinetic and interaction energy terms of the Hamiltonian are treated similarly together, and are provided by the same positive semidefinite expression. For this reason, non-linear fermionic contributions are used in block operators from which the positive semidefinite forms are constructed. The transformation is possible to be done when a system of nonlinear equations, called matching equations, are satisfied. The procedure of solving the matching equations is also indicated.

*Key-Words:* Non-integrable many-body systems, Hamiltonian in positive semidefinite form, exact ground states

## 1 Introduction

### 1.1 About exact results in quantum theory of many-body systems

Exact theoretical results represent milestones in physics [1] since based on them, it is possible to test approximations, to probe numerical codes, to evaluate model predictions, approach qualities, or physical interpolations, extend or develop model descriptions by comparison to experiment, or even to test the quality of a given theoretical model. Starting from these premises, techniques providing exact results for physical systems have an extremely broad literature and a livelong history. Since in our neighborhood many-body systems abound, and their behavior in most cases is embedded even at room temperature in quantum mechanics, such cases attract main interest, hence the majority of methods have been developed for quantum mechanical many-body systems, e.g. electrons [2].

However, till now, in the development of techniques providing exact results, mainly only integrable models were considered [1, 2]. The integrability is a model property, which enhances the deduction of complete exact solutions by requiring supplementary constrains to the model. These constrains, in a simple view, demand an equal number of degrees of freedom

( $N_{df}$ ) and constants of motion ( $N_{cm}$ ) [3, 4]. However, in the majority of many-body cases,  $N_{df}$  (e.g. the independent  $\mathbf{r}$ -space coordinates), as order of magnitude is around the Avogadro's number  $N_{df} \sim 6 \cdot 10^{26}$ , and contrary to this,  $N_{cm}$  (e.g. energy, the components of the total momentum, and total angular momentum) usually attain  $N_{cm} \sim \mathcal{O}(10)$ . Consequently, integrable systems are extremely rare, and mostly only one dimensional special models are placed in this category. Because of this reason, 99% of the many-body systems in nature are non-integrable, hence a strong demand is present for techniques able to provide exact results for non-integrable systems.

### 1.2 Exact results for non-integrable systems: positive semidefinite operator technique

However exact results for non-integrable systems have been deduced by other means as well [5], the method based on positive semidefinite operator properties seems to be one of the most successful techniques (for an extended review see [6, 7]). The interest for positive semidefinite operators in the field goes back several decades [8], the method had several preliminary versions connecting also the variational principle in the procedure [9, 10, 11, 12], but in the current version which concentrates on a fixed given system, the

technique casts first the system Hamiltonian ( $\hat{H}$ ) in a positive semidefinite form  $\hat{H} = \hat{P} + C$ , where  $\hat{P}$  is a positive semidefinite operator and  $C$  a scalar, and obtains the exact ground state by deducing the most general Hilbert space vector  $|\Phi_g\rangle$  which satisfies the equation  $\hat{P}|\Phi_g\rangle = 0$ . This technique has lead to exact result in circumstances unimaginable befor in the context of exact solutions, as in the case of two [13] and three-dimensional [14] strongly interacting electron systems, disordered systems in two dimensions [15], delocalization effects in two dimension [16], stripes or droplets in two dimensions [17], interaction-created effective bands [18], or exact results for different non-integrable chain structures [19, 20, 21].

Besides its success, the technique is still in extensive development, being far from a complete and closed method, whose know-how informations are all well known. For example, up to this moment, the transformation of the kinetic energy ( $\hat{H}_{kin}$ ) and interaction energy ( $\hat{H}_{int}$ ) parts of  $\hat{H}$  in positive semidefinite forms has been separately performed, the obtained results restricting in this manner the parameter space regions and the type of ground state wave functions that were possible to be covered. In the present work we correct this inconvenience, and demonstrate that it is possible to chose positive semidefinite operators such to obtaint simultaneously both the  $\hat{H}_{kin}$  and  $\hat{H}_{int}$  terms of the Hamiltonian from the same expression in exact terms.

The remaining part of the paper is constructed as follows: Section 2 presents the studied system and its Hamiltonian, Section 3 introduces the used block operators and defines the matching equations, Section 4 presents the transformation in positive semidefinite form, Section 5 specifies how the matching equations preserving the transformation can be solved, and finally, Section 6, containing the summary and conclusions closes the presentation.

## 2 The system under consideration

The analyzed system is a quadrilateral chain with external hoppings. The unit cell of the system has three sites:  $\mathbf{j}_n, \mathbf{j}_n + \mathbf{r}_1, \mathbf{j}_n + \mathbf{r}_2$ , and the chain is obtained by translating a given site  $\mathbf{i}$  by the Bravais vector  $\mathbf{a}$ , hence  $\mathbf{j}_n = \mathbf{i} + n\mathbf{a}$ . The obtained system has  $N_c$  cells, and periodic boundary conditions are used, i.e.  $\mathbf{j}_{N_c+1} = \mathbf{i}$ . The chain is considered quantum mechanical, and the Hamiltonian, written in second quantized form, is defined as follows

**Definition 1** *The system Hamiltonian  $\hat{H} = \hat{H}_{kin} + \hat{H}_{int}$  is defined of Hubbard type, containing in the kinetic energy term  $\hat{H}_{kin}$  hopping contributions  $t_{\mathbf{j}_2, \mathbf{j}_1}$*

*from an arbitrary site  $\mathbf{j}_1$  to an arbitrary nearest-neighbor site  $\mathbf{j}_2$ , and on-site one-particle potentials  $\epsilon_{\mathbf{j}}$  at each site  $\mathbf{j}$ . The interaction energy term  $\hat{H}_{int}$  contains only contributions given by the local Coulomb repulsion  $U_{\mathbf{j}} \geq 0$  at each site  $\mathbf{j}$ .*

Written in explicit terms one has

$$\begin{aligned} \hat{H} = \sum_{\mathbf{i}, \sigma} \{ & t_1 (\hat{c}_{\mathbf{i}, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{a}, \sigma} + \\ & \hat{c}_{\mathbf{i}+\mathbf{a}, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma} + \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma}) + t_2 (\hat{c}_{\mathbf{i}-\mathbf{a}, \mathbf{r}_1, \sigma}^\dagger \times \\ & \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \hat{c}_{\mathbf{i}-\mathbf{a}, \mathbf{r}_2, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma}) + H.c.] + (\epsilon_1 \hat{n}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \\ & \epsilon_2 \hat{n}_{\mathbf{i}+\mathbf{r}_2, \sigma} + \epsilon_0 \hat{n}_{\mathbf{i}, \sigma}) \} + \sum_{\mathbf{i}} (U_1 \hat{n}_{\mathbf{i}+\mathbf{r}_1, \sigma} \hat{n}_{\mathbf{i}+\mathbf{r}_1, -\sigma} + \\ & U_2 \hat{n}_{\mathbf{i}+\mathbf{r}_2, \sigma} \hat{n}_{\mathbf{i}+\mathbf{r}_2, -\sigma} + U_0 \hat{n}_{\mathbf{i}, \sigma} \hat{n}_{\mathbf{i}, -\sigma}). \end{aligned} \quad (1)$$

In this expression  $\hat{c}_{\mathbf{j}, \sigma}^\dagger$ , ( $\hat{c}_{\mathbf{j}, \sigma}$ ), creates, (annihilates) an electron with  $\sigma$  spin projection at the site  $\mathbf{j}$ , and  $\hat{n}_{\mathbf{j}, \sigma} = \hat{c}_{\mathbf{j}, \sigma}^\dagger \hat{c}_{\mathbf{j}, \sigma}$  is the particle number operator. The  $t_1 = t_{\mathbf{i}+\mathbf{r}_1, \mathbf{i}} = t_{\mathbf{i}+\mathbf{r}_2, \mathbf{i}}$  and  $t_2 = t_{\mathbf{i}+\mathbf{r}_1, \mathbf{i}+\mathbf{a}+\mathbf{r}_1} = t_{\mathbf{i}+\mathbf{r}_2, \mathbf{i}+\mathbf{a}+\mathbf{r}_2}$  parameters are hopping matrix elements,  $\epsilon_m = \epsilon_{\mathbf{i}+\mathbf{r}_m}$  with  $m = 0, 1, 2$  and convention  $\mathbf{r}_0 = 0$  are one-particle on-site potentials, while  $U_m = U_{\mathbf{i}+\mathbf{r}_m}$  represent the on-site local Coulomb repulsion values. The physical parameters in each cell are considered the same, and since the  $\hat{c}_{\mathbf{j}, \sigma}$  operators are fermionic, they satisfy standard canonical anticommutation rules.

## 3 Preliminaries for the transformation of the Hamiltonian

### 3.1 The used block operators

For each cell defined at an arbitrary lattice site  $\mathbf{i}$  one introduces 9 block operators containing each besides linear terms also nonlinear fermionic operator contributions acting on the sites of the block. One has

**Definition 2** *The nine block operators defined at fixed but arbitrary spin projection  $\sigma$  for each cell at the site  $\mathbf{i}$  are linear combinations of all site contributions  $\mathcal{S}_{\mathbf{j}, \sigma}$  present in the block, a given site contribution being of the form  $\mathcal{S}_{\mathbf{j}, \sigma} = (\alpha \hat{c}_{\mathbf{j}, \sigma} + \alpha_n \hat{c}_{\mathbf{j}, \sigma} \hat{n}_{\mathbf{j}, -\sigma})$ , where  $\alpha, \alpha_n$  are numerical coefficients. Given by the second term in  $\mathcal{S}_{\mathbf{j}, \sigma}$ , the introduced block operators are non-linear expressions of the canonical Fermi operators.*

For the explicit expressions of the defined block operators one has

$$\begin{aligned} \hat{A}_{\mathbf{i}, \sigma} = & (a_1 \hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2, \sigma} + a_{1, n} \hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2, \sigma} \hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2, -\sigma}) + \\ & (a_2 \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma} + a_{2, n} \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma} \hat{n}_{\mathbf{i}+\mathbf{r}_2, -\sigma}) + (a_3 \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \\ & a_{3, n} \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma} \hat{n}_{\mathbf{i}+\mathbf{r}_1, -\sigma}) + (a_4 \hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1, \sigma} + a_{4, n} \hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1, \sigma} \end{aligned}$$

$$\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,-\sigma})(a_5\hat{c}_{\mathbf{i},\sigma} + a_{5,n}\hat{c}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i},-\sigma}),$$

$$\begin{aligned} \hat{B}_{\mathbf{i},\sigma} = & (b_3\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} + b_{3,n}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_1,-\sigma}) + \\ & (b_4\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma} + b_{4,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,-\sigma}) + \\ & (b_5\hat{c}_{\mathbf{i},\sigma} + b_{5,n}\hat{c}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i},-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{C}_{\mathbf{i},\sigma} = & (c_1\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma} + c_{1,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,-\sigma}) + \\ & (c_2\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} + c_{2,n}\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_2,-\sigma}) + \\ & (c_5\hat{c}_{\mathbf{i},\sigma} + c_{5,n}\hat{c}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i},-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{D}_{\mathbf{i},\sigma} = & (d_1\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma} + d_{1,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,-\sigma}) + \\ & (d_4\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma} + d_{4,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,-\sigma}) + \\ & (d_5\hat{c}_{\mathbf{i},\sigma} + d_{5,n}\hat{c}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i},-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{E}_{\mathbf{i},\sigma} = & (e_2\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} + e_{2,n}\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_2,-\sigma}) + \\ & (e_3\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} + e_{3,n}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_1,-\sigma}) + \\ & (e_5\hat{c}_{\mathbf{i},\sigma} + e_{5,n}\hat{c}_{\mathbf{i},\sigma}\hat{n}_{\mathbf{i},-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{F}_{\mathbf{i},\sigma} = & (f_2\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} + f_{2,n}\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_2,-\sigma}) + \\ & (f_3\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} + f_{3,n}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_1,-\sigma}) + (f_4\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma} + \\ & f_{4,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{G}_{\mathbf{i},\sigma} = & (g_1\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma} + g_{1,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,-\sigma}) + \\ & (g_2\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} + g_{2,n}\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_2,-\sigma}) + \\ & (g_3\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} + g_{3,n}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_1,-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{H}_{\mathbf{i},\sigma} = & (h_1\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma} + h_{1,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,-\sigma}) + \\ & (h_2\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma} + h_{2,n}\hat{c}_{\mathbf{i}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_2,-\sigma}) + \\ & (h_4\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma} + h_{4,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,-\sigma}), \end{aligned}$$

$$\begin{aligned} \hat{J}_{\mathbf{i},\sigma} = & (j_1\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma} + j_{1,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2,-\sigma}) + \\ & (j_3\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma} + j_{3,n}\hat{c}_{\mathbf{i}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}+\mathbf{r}_1,-\sigma}) + \\ & (j_4\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma} + j_{4,n}\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,\sigma}\hat{n}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1,-\sigma}). \end{aligned} \quad (2)$$

As can be seen, one has 8 block operators defined on different triangles, and one block operator defined on a quadrilater containing a site also in its middle. The 9 block operators contain totally 58 coefficients, i.e. block operator parameters. We note that the block operator coefficients are indexed by the in-cell site index  $\ell$  of the site to which they are connected. The possible in-cell notations  $\ell = 1, 2, 3, 4, 5$  correspond in order to the sites  $\mathbf{i} - \mathbf{a} + \mathbf{r}_2, \mathbf{i} + \mathbf{r}_2, \mathbf{i} + \mathbf{r}_1, \mathbf{i} - \mathbf{a} + \mathbf{r}_1, \mathbf{i}$ .

We would like to note that the blocks are not randomly chosen, but with a well defined strategy. On this line we mention that, the block operators  $\hat{B}_{m,\mathbf{i},\sigma}$ , where  $m$  is a discrete index (i.e. in our

case  $m = 1, 2, \dots, 9$ , for which  $\hat{B}$  becomes in order  $\mathcal{A}, \mathcal{B}, \mathcal{D}, \dots, \mathcal{J}$ ), are introduced with the aim to construct positive semidefinite operators from them. Indeed  $\hat{P}_{m,\mathbf{i},\sigma} = \hat{B}_{m,\mathbf{i},\sigma}^\dagger \hat{B}_{m,\mathbf{i},\sigma}$  are positive semidefinite operators. The blocks are such chosen to lead in the explicit expression of  $\hat{P}_{m,\mathbf{i},\sigma}$  (obtained after effectively calculating the product  $\hat{B}_{m,\mathbf{i},\sigma}^\dagger \hat{B}_{m,\mathbf{i},\sigma}$ ) to terms of the form present in the starting Hamiltonian (1). That is why higher blocks as those present in (2) are missing, since long-range hopping terms are not present in (1). Furthermore, even if care is taken while choosing the blocks  $\hat{B}_{m,\mathbf{i},\sigma}$  as specified above, several, called correlated hopping terms (i.e. terms of the form  $\hat{c}_{\mathbf{j}_1,\sigma}^\dagger \hat{c}_{\mathbf{j}_2,\sigma} \hat{n}_{\mathbf{j}_1,-\sigma}, \hat{c}_{\mathbf{j}_1,\sigma}^\dagger \hat{c}_{\mathbf{j}_2,\sigma} \hat{n}_{\mathbf{j}_2,-\sigma}, \hat{c}_{\mathbf{j}_1,\sigma}^\dagger \hat{c}_{\mathbf{j}_2,\sigma} \hat{n}_{\mathbf{j}_1,-\sigma} \hat{n}_{\mathbf{j}_2,-\sigma}$ ) missing in (1) emerge from the expression of  $\hat{P}_{m,\mathbf{i},\sigma}$ . These are present on bonds  $(\mathbf{j}_1, \mathbf{j}_2)$ , and in order to eliminate these contributions (since are not present into the starting  $\hat{H}$ ), one needs at least three different block operators to provide contributions on the same bond. This condition fixes the number of blocks to 9.

It is important to underline that the  $\alpha_n \hat{c}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma}$  non-linear fermionic contribution is present in block operators inside the  $\mathcal{S}_{\mathbf{j},\sigma}$  term, because via  $\hat{P}_{m,\mathbf{i},\sigma}$  it reproduces the interaction part of the Hamiltonian. Indeed, for example the product  $\hat{B}_{m,\mathbf{i},\sigma}^\dagger \hat{B}_{m,\mathbf{i},\sigma}$  leads to terms of the form  $(\alpha_n \hat{c}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma})^\dagger (\alpha_n \hat{c}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma}) = |\alpha_n|^2 \hat{n}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma}$ , whose operator  $\hat{n}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma}$  exactly coincides to the form of the interaction energy operator in  $\hat{H}$ . Consequently, the presence of the non-linear contributions  $\alpha_n \hat{c}_{\mathbf{j},\sigma} \hat{n}_{\mathbf{j},-\sigma}$  in block operators opens the doors for reproducing simultaneously both the kinetic and interaction parts of the Hamiltonian from the same positive semidefinite form.

### 3.2 The matching equations

Let us start by defining the equations under discussion, called matching equations.

**Definition 3** *Matching equations are equalities connecting the parameters of the starting Hamiltonian to the parameters of the block operators. These equalities arise from collecting from  $\hat{P} = \sum_{m,\mathbf{i},\sigma} \hat{P}_{m,\mathbf{i},\sigma}$  all contributions which provide the same operator  $\hat{O}_n$  present in the expression of  $\hat{H}$  from (1) as well. If in  $\hat{P}$ , a given collected operator  $\hat{O}_n$  gives rise to the contribution  $V_{n,block} \hat{O}_n$ , where  $V_{n,block}$  is a scalar depending on block operator parameters, and the same operator  $\hat{O}_n$  appears in (1) as  $W_{n,H} \hat{O}_n$ , where the scalar  $W_{n,H}$  depends on the Hamiltonian parameters, than the  $n$ -th matching equation is given by the equality  $V_{n,block} = W_{n,H}$ .*

Taking into account all contributions present in  $\hat{P}$ , one finds 42 matching equations as follows

$$\begin{aligned}
& a_3^* a_5 + b_3^* b_5 + e_3^* e_5 = t_{3,5} = t_1, \\
& a_{3,n}^* a_5 + b_{3,n}^* b_5 + e_{3,n}^* e_5 = 0, \\
& a_3^* a_{5,n} + b_3^* b_{5,n} + e_3^* e_{5,n} = 0, \\
& a_{3,n}^* a_{5,n} + b_{3,n}^* b_{5,n} + e_{3,n}^* e_{5,n} = 0, \\
& a_4^* a_5 + b_4^* b_5 + d_4^* d_5 = t_{4,5} = t_1, \\
& a_{4,n}^* a_5 + b_{4,n}^* b_5 + d_{4,n}^* d_5 = 0, \\
& a_4^* a_{5,n} + b_4^* b_{5,n} + d_4^* d_{5,n} = 0, \\
& a_{4,n}^* a_{5,n} + b_{4,n}^* b_{5,n} + d_{4,n}^* d_{5,n} = 0, \\
& a_1^* a_5 + c_1^* c_5 + d_1^* d_5 = t_{1,5} = t_1, \\
& a_{1,n}^* a_5 + c_{1,n}^* c_5 + d_{1,n}^* d_5 = 0, \\
& a_1^* a_{5,n} + c_1^* c_{5,n} + d_1^* d_{5,n} = 0, \\
& a_{1,n}^* a_{5,n} + c_{1,n}^* c_{5,n} + d_{1,n}^* d_{5,n} = 0, \\
& a_2^* a_5 + c_2^* c_5 + e_2^* e_5 = t_{2,5} = t_1, \\
& a_{2,n}^* a_5 + c_{2,n}^* c_5 + e_{2,n}^* e_5 = 0, \\
& a_2^* a_{5,n} + c_2^* c_{5,n} + e_2^* e_{5,n} = 0, \\
& a_{2,n}^* a_{5,n} + c_{2,n}^* c_{5,n} + e_{2,n}^* e_{5,n} = 0, \\
& a_3^* a_4 + b_3^* b_4 + f_3^* f_4 + j_3^* j_4 = t_{3,4} = t_2, \\
& a_{3,n}^* a_4 + b_{3,n}^* b_4 + f_{3,n}^* f_4 + j_{3,n}^* j_4 = 0, \\
& a_3^* a_{4,n} + b_3^* b_{4,n} + f_3^* f_{4,n} + j_3^* j_{4,n} = 0, \\
& a_{3,n}^* a_{4,n} + b_{3,n}^* b_{4,n} + f_{3,n}^* f_{4,n} + j_{3,n}^* j_{4,n} = 0, \\
& a_2^* a_1 + c_2^* c_1 + g_2^* g_1 + h_2^* h_1 = t_{2,1} = t_2, \\
& a_{2,n}^* a_1 + c_{2,n}^* c_1 + g_{2,n}^* g_1 + h_{2,n}^* h_1 = 0, \\
& a_2^* a_{1,n} + c_2^* c_{1,n} + g_2^* g_{1,n} + h_2^* h_{1,n} = 0, \\
& a_{2,n}^* a_{1,n} + c_{2,n}^* c_{1,n} + g_{2,n}^* g_{1,n} + h_{2,n}^* h_{1,n} = 0, \\
& a_2^* a_3 + a_1^* a_4 + d_1^* d_4 + e_2^* e_3 + f_2^* f_3 + \\
& \quad g_2^* g_3 + h_1^* h_4 + j_1^* j_4 = t_{2,3} = t_{\perp} = 0, \\
& a_{2,n}^* a_3 + a_{1,n}^* a_4 + d_{1,n}^* d_4 + e_{2,n}^* e_3 + \\
& \quad f_{2,n}^* f_3 + g_{2,n}^* g_3 + h_{1,n}^* h_4 + j_{1,n}^* j_4 = 0, \\
& a_2^* a_{3,n} + a_1^* a_{4,n} + d_1^* d_{4,n} + e_2^* e_{3,n} + \\
& \quad f_2^* f_{3,n} + g_2^* g_{3,n} + h_1^* h_{4,n} + j_1^* j_{4,n} = 0, \\
& a_{2,n}^* a_{3,n} + a_{1,n}^* a_{4,n} + d_{1,n}^* d_{4,n} + e_{2,n}^* e_{3,n} + \\
& \quad f_{2,n}^* f_{3,n} + g_{2,n}^* g_{3,n} + h_{1,n}^* h_{4,n} + j_{1,n}^* j_{4,n} = 0, \\
& a_3^* a_1 + g_3^* g_1 + j_3^* j_1 = t_{3,1} = 0, \\
& a_{3,n}^* a_1 + g_{3,n}^* g_1 + j_{3,n}^* j_1 = 0, \\
& a_3^* a_{1,n} + g_3^* g_{1,n} + j_3^* j_{1,n} = 0,
\end{aligned}$$

$$a_{3,n}^* a_{1,n} + g_{3,n}^* g_{1,n} + j_{3,n}^* j_{1,n} = 0,$$

$$a_4^* a_2 + f_4^* f_2 + h_4^* h_2 = t_{4,2} = 0,$$

$$a_{4,n}^* a_2 + f_{4,n}^* f_2 + h_{4,n}^* h_2 = 0,$$

$$a_4^* a_{2,n} + f_4^* f_{2,n} + h_4^* h_{2,n} = 0,$$

$$a_{4,n}^* a_{2,n} + f_{4,n}^* f_{2,n} + h_{4,n}^* h_{2,n} = 0,$$

$$\epsilon_0 = |a_5|^2 + |b_5|^2 + |c_5|^2 + |d_5|^2 + |e_5|^2 - p,$$

$$\epsilon_1 = |a_3|^2 + |a_4|^2 + |b_3|^2 + |b_4|^2 + |d_4|^2 + |e_3|^2 + |f_3|^2 + |f_4|^2 + |g_3|^2 + |j_3|^2 + |j_4|^2 + |h_4|^2 - p,$$

$$\epsilon_2 = |a_1|^2 + |a_2|^2 + |c_1|^2 + |c_2|^2 + |d_1|^2 + |e_2|^2 + |g_1|^2 + |g_2|^2 + |f_2|^2 + |h_1|^2 + |h_2|^2 + |j_1|^2 - p,$$

$$\begin{aligned}
U_1 = 2[ & (a_3^* a_{3,n} + a_{3,n}^* a_3 + |a_{3,n}|^2) + \\
& (a_4^* a_{4,n} + a_{4,n}^* a_4 + |a_{4,n}|^2) + (b_3^* b_{3,n} + \\
& b_{3,n}^* b_3 + |b_{3,n}|^2) + (b_4^* b_{4,n} + b_{4,n}^* b_4 + \\
& |b_{4,n}|^2) + (d_4^* d_{4,n} + d_{4,n}^* d_4 + |d_{4,n}|^2) + \\
& (e_3^* e_{3,n} + e_{3,n}^* e_3 + |e_{3,n}|^2) + (f_3^* f_{3,n} + \\
& f_{3,n}^* f_3 + |f_{3,n}|^2) + (f_4^* f_{4,n} + f_{4,n}^* f_4 + \\
& |f_{4,n}|^2) + (g_3^* g_{3,n} + g_{3,n}^* g_3 + |g_{3,n}|^2) + \\
& (j_4^* j_{4,n} + j_{4,n}^* j_4 + |j_{4,n}|^2) + (j_3^* j_{3,n} + \\
& j_{3,n}^* j_3 + |j_{3,n}|^2) + (h_4^* h_{4,n} + h_{4,n}^* h_4 + \\
& |h_{4,n}|^2)],
\end{aligned}$$

$$\begin{aligned}
U_2 = 2[ & (a_1^* a_{1,n} + a_{1,n}^* a_1 + |a_{1,n}|^2) + \\
& (a_2^* a_{2,n} + a_{2,n}^* a_2 + |a_{2,n}|^2) + (c_1^* c_{1,n} + \\
& c_{1,n}^* c_1 + |c_{1,n}|^2) + (c_2^* c_{2,n} + c_{2,n}^* c_2 + \\
& |c_{2,n}|^2) + (d_1^* d_{1,n} + d_{1,n}^* d_1 + |d_{1,n}|^2) + \\
& (e_2^* e_{2,n} + e_{2,n}^* e_2 + |e_{2,n}|^2) + (g_2^* g_{2,n} + \\
& g_{2,n}^* g_2 + |g_{2,n}|^2) + (g_1^* g_{1,n} + g_{1,n}^* g_1 + \\
& |g_{1,n}|^2) + (f_2^* f_{2,n} + f_{2,n}^* f_2 + |f_{2,n}|^2) + \\
& (h_1^* h_{1,n} + h_{1,n}^* h_1 + |h_{1,n}|^2) + (h_2^* h_{2,n} + \\
& h_{2,n}^* h_2 + |h_{2,n}|^2) + (j_1^* j_{1,n} + j_{1,n}^* j_1 + \\
& |j_{1,n}|^2)],
\end{aligned}$$

$$\begin{aligned}
U_0 = 2[ & (a_5^* a_{5,n} + a_{5,n}^* a_5 + |a_{5,n}|^2) + \\
& (b_5^* b_{5,n} + a_{b,n}^* b_5 + |b_{5,n}|^2) + (c_5^* c_{5,n} + \\
& c_{5,n}^* c_5 + |c_{5,n}|^2) + (d_5^* d_{5,n} + d_{5,n}^* d_5 + \\
& |d_{5,n}|^2) + (e_5^* e_{5,n} + e_{5,n}^* e_5 + |e_{5,n}|^2)]. \quad (3)
\end{aligned}$$

Some observations must be added to Eq.(3). First, group of four equations are connected to different

bonds in the first 36 equations (i.e. 9 group of 4 equations connected to 9 different bonds). The hopping matrix elements  $t_{\mathbf{j}_2, \mathbf{j}_1}$  along the bonds  $(\mathbf{j}_2, \mathbf{j}_1)$  are denoted for simplicity by  $t_{\ell(\mathbf{j}_2), \ell(\mathbf{j}_1)} = t_{\mathbf{j}_2, \mathbf{j}_1}$ , so the in-cell  $\ell$  index of the sites  $\mathbf{j}_2$  and  $\mathbf{j}_1$  (e.g. in the first line of (3),  $t_1 = t_{\mathbf{i}+\mathbf{r}_1, \mathbf{i}} = t_{3,5}$ , etc.). Second, for reasons which will be clarified in the next section, the on-site Hamiltonian contributions are considered  $\epsilon'_n = \epsilon_n + p$  instead  $\epsilon_n$  present in the starting Hamiltonian from Eq.(1), see Eq.(7).

#### 4 The transformation of the Hamiltonian in positive semidefinite form

Given by the nonlinear structure of the block operators, both the kinetic and the interacting part of the Hamiltonian will be contained in the same positive semidefinite operators after the exact transformation of the Hamiltonian in positive semidefinite form. In order to show this, first we analyze a Lemma.

**Lemma 4** *All Hamiltonians describing physical systems can be written in positive semidefinite form  $\hat{H} = \hat{P} + C$ , where  $\hat{P}$  is a positive semidefinite operator and  $C$  a constant scalar.*

**Proof:** Indeed, all Hamiltonians describing physical systems have a spectrum bounded below [22]. The lower bound of the spectrum is the ground state energy  $E_g$ , hence, since do not has negative eigenvalues, the operator  $\hat{H} - E_g$  is positive semidefinite, i.e.  $\hat{H} - E_g = \hat{P}$ , where  $\hat{P}$  is a positive semidefinite operator. Furthermore  $E_g = C$  is a scalar, consequently  $\hat{H} = \hat{P} + C$  holds. Q.E.D.

**Theorem 5** *At constant number of total electrons  $N$ , and if the matching equations (3) hold (and allow solutions) the Hamiltonian from Eq.(1) can be exactly transformed in the positive semidefinite form*

$$\hat{H} = \hat{P} - p\hat{N}, \quad (4)$$

where  $\hat{N} = \sum_{\mathbf{i}, \sigma} \hat{n}_{\mathbf{i}, \sigma}$  represents the operator of the total number of electrons,  $p$  is a scalar, and the positive semidefinite operator  $\hat{P}$  has the form

$$\begin{aligned} \hat{P} = & \sum_{\mathbf{i}, \sigma} [\hat{A}_{\mathbf{i}, \sigma}^\dagger \hat{A}_{\mathbf{i}, \sigma} + \hat{B}_{\mathbf{i}, \sigma}^\dagger \hat{B}_{\mathbf{i}, \sigma} + \hat{C}_{\mathbf{i}, \sigma}^\dagger \hat{C}_{\mathbf{i}, \sigma} \\ & + \hat{D}_{\mathbf{i}, \sigma}^\dagger \hat{D}_{\mathbf{i}, \sigma} + \hat{E}_{\mathbf{i}, \sigma}^\dagger \hat{E}_{\mathbf{i}, \sigma} + \hat{F}_{\mathbf{i}, \sigma}^\dagger \hat{F}_{\mathbf{i}, \sigma} + \hat{G}_{\mathbf{i}, \sigma}^\dagger \hat{G}_{\mathbf{i}, \sigma} \\ & + \hat{H}_{\mathbf{i}, \sigma}^\dagger \hat{H}_{\mathbf{i}, \sigma} + \hat{J}_{\mathbf{i}, \sigma}^\dagger \hat{J}_{\mathbf{i}, \sigma}]. \end{aligned} \quad (5)$$

**Proof:** First, given by Lemma 1, since describes a physical system, the Hamiltonian from Eq.(1) can be

transformed in positive semidefinite form  $\hat{H} = \hat{P} + C$ . One shows below that  $C$  is of the form  $C = -pN$  and  $\hat{P}$  is of the form (5).

i) We observe that since the total number of electrons in the system is a constant number  $N$  (i.e.  $\hat{N}$  is a constant of motion, hence commutes with  $\hat{H}$ ), all eigenfunctions of  $\hat{H}$ , namely  $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$  provide the same eigenvalue  $N$  for  $\hat{N}$  via  $\hat{N}|\Psi_n\rangle = N|\Psi_n\rangle$ . Furthermore, since the eigenvectors of  $\hat{H}$  build up a base  $\{|\Psi_n\rangle\}$  for the Hilbert space of the problem, all normalized wave vectors  $|\Psi\rangle = \sum_n c_n |\Psi_n\rangle$ , where  $c_n$  are numerical coefficients, provide  $\hat{N}|\Psi\rangle = N|\Psi\rangle$ , hence  $\hat{N}$  can be changed to  $N$ . Consequently in (4),  $C = -pN$  holds.

ii) From Eq.(4) is seen that  $\hat{P} = \hat{H} + p\hat{N}$ . Taking into account the expression of  $\hat{N}$  given in Theorem 5, and expression of  $\hat{H}$  in (1) one obtains

$$\begin{aligned} \hat{H} + p\hat{N} = & \sum_{\mathbf{i}, \sigma} \{ [t_1 (\hat{c}_{\mathbf{i}, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{a}, \sigma} + \\ & \hat{c}_{\mathbf{i}+\mathbf{a}, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma} + \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma}) + t_2 (\hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_1, \sigma}^\dagger \times \\ & \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \hat{c}_{\mathbf{i}-\mathbf{a}+\mathbf{r}_2, \sigma}^\dagger \hat{c}_{\mathbf{i}+\mathbf{r}_2, \sigma}) + H.c.] + (\epsilon'_1 \hat{n}_{\mathbf{i}+\mathbf{r}_1, \sigma} + \\ & \epsilon'_2 \hat{n}_{\mathbf{i}+\mathbf{r}_2, \sigma} + \epsilon'_0 \hat{n}_{\mathbf{i}, \sigma}) \} + \sum_{\mathbf{i}} (U_1 \hat{n}_{\mathbf{i}+\mathbf{r}_1, \sigma} \hat{n}_{\mathbf{i}+\mathbf{r}_1, -\sigma} + \\ & U_2 \hat{n}_{\mathbf{i}+\mathbf{r}_2, \sigma} \hat{n}_{\mathbf{i}+\mathbf{r}_2, -\sigma} + U_0 \hat{n}_{\mathbf{i}, \sigma} \hat{n}_{\mathbf{i}, -\sigma}), \end{aligned} \quad (6)$$

where  $\epsilon'_m = \epsilon_m + p$ , and  $m = 0, 1, 2$ . Consequently, if we introduce the notation  $\hat{H} \equiv \hat{H}(\epsilon_m)$ , then simply  $\hat{H} + p\hat{N} \equiv \hat{H}(\epsilon'_m)$  holds, and the transformation in Eq.(4) means in fact

$$\hat{H}(\epsilon'_m) = \hat{P}. \quad (7)$$

But the matching equations from Eq.(3) have been constructed exactly based on the equality (7). Indeed, effectuating the calculations in the right side of (5) and taking into account (3) we recover the equality (7). For example the operator  $\hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma}$  which represents the hopping along the bond  $\mathbf{i} + \mathbf{r}_1, \mathbf{i}$  described in  $\hat{H}$  by the hopping matrix element  $t_{3,5} = t_1$ , emerges in  $\hat{P}$  only from three contributions, namely: from  $\hat{A}_{\mathbf{i}, \sigma}^\dagger \hat{A}_{\mathbf{i}, \sigma}$ , with the coefficient  $a_3^* a_5$ ; from  $\hat{B}_{\mathbf{i}, \sigma}^\dagger \hat{B}_{\mathbf{i}, \sigma}$ , with coefficient  $b_3^* b_5$ ; and finally from  $\hat{E}_{\mathbf{i}, \sigma}^\dagger \hat{E}_{\mathbf{i}, \sigma}$ , with coefficient  $e_3^* e_5$ . Using the notations of Definition 3, one has for  $\hat{O}_n = \hat{c}_{\mathbf{i}+\mathbf{r}_1, \sigma}^\dagger \hat{c}_{\mathbf{i}, \sigma}$  the expressions  $V_{n, block} = a_3^* a_5 + b_3^* b_5 + e_3^* e_5$ ,  $W_{n, H} = t_{3,5} = t_1$ , consequently, from the equality  $V_{n, block} = W_{n, H}$  one finds the matching equation  $a_3^* a_5 + b_3^* b_5 + e_3^* e_5 = t_1$ , which is placed on the first row of (3). The following three rows are related to the correlated hopping terms along the same bond, of the form

$\hat{O}_{n_1} = \hat{c}_{i+r_1,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{n}_{i+r_1,-\sigma}$ ,  $\hat{O}_{n_2} = \hat{c}_{i+r_1,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{n}_{i,-\sigma}$ , and  $\hat{O}_{n_3} = \hat{c}_{i+r_1,\sigma}^\dagger \hat{c}_{i,\sigma} \hat{n}_{i+r_1,-\sigma} \hat{n}_{i,-\sigma}$ . The corresponding  $V$  value of these contributions in order becomes  $V_{n_1,block} = a_{3,n}^* a_5 + b_{3,n}^* b_5 + e_{3,n}^* e_5$ ,  $V_{n_2,block} = a_{3,n}^* a_{5,n} + b_{3,n}^* b_{5,n} + e_{3,n}^* e_{5,n}$ , and  $V_{n_3,block} = a_{3,n}^* a_{5,n} + b_{3,n}^* b_{5,n} + e_{3,n}^* e_{5,n}$ . Since such type of correlation hopping operators are missing from the Hamiltonian (1), one has  $W_{n_1,H} = W_{n_2,H} = W_{n_3,H} = 0$ , hence the second, third and fourth rows of (3) arise. All equalities from (3) are similarly obtained. Q.E.D.

## 5 How the matching equations can be solved

The transformation (4) can be effectively used if the block operator parameters, together with the scalar  $p$  are explicitly known. For this to be possible, we must solve the matching equations. These, present in (3), are coupled non-linear equations whose unknown variables are the block operator parameters and  $p$ , while whose known variables are the parameters of the starting  $\hat{H}$  in (1), namely the  $t_1, t_2, \epsilon_m, U_m$ ,  $m = 0, 1, 2$  values. Since it is difficult to provide solutions for a huge coupled non-linear system of equations as (3), below we indicate how this can be done.

In order to provide solutions for (3) we used a stochastic numerical code. This works as follows: 26 block operator parameters, namely

$$\begin{aligned} & a_5, b_5, e_5, e_3, a_{3,n}, b_{3,n}, a_{5,n}, b_{5,n}, d_4, d_5, \\ & a_{4,n}, b_{4,n}, a_{1,n}, c_{1,n}, d_{1,n}, d_1, e_2, c_{2,n}, g_1, \\ & g_3, j_1, g_{3,n}, f_2, f_4, h_2, f_{4,n}, \end{aligned} \quad (8)$$

are statistically generated. Once numbers are given to the parameters from (8), the rows 1-24 together with the rows 29-36 of (3) become together a block diagonal non-homogenous linear system of equations, from which the remaining 32 block operator parameters can be deduced, namely

$$\begin{aligned} & a_3, b_3, e_{3,n}, e_{5,n}, \\ & a_4, b_4, d_{4,n}, d_{5,n}, \\ & a_1, c_1, c_5, c_{5,n}, \\ & a_2, c_2, e_{2,n}, a_{2,n}, \\ & j_3, j_{1,n}, j_{3,n}, g_{1,n}, \\ & h_4, h_{4,n}, f_{2,n}, h_{2,n}, \\ & g_2, h_1, g_{2,n}, h_{1,n}, \\ & f_3, j_4, f_{3,n}, j_{4,n}. \end{aligned} \quad (9)$$

Because of the block diagonal nature mentioned above, in order, each row of (9) can be deduced only from 4 linear non-homogenous equations provided by

(3) as follows: the first line of (9), from the 4 equations related to  $t_{3,5}$  [lines 1-4 from (3)]; the second line of (9), from the 4 equations related to  $t_{4,5}$  [lines 5-8 from (3)]; the third line of (9), from the 4 equations related to  $t_{1,5}$  [lines 9-12 from (3)]; the fourth line of (9), from the 4 equations related to  $t_{2,5}$  [lines 13-16 from (3)]; the fifth line of (9), from the 4 equations related to  $t_{3,1}$  [lines 29-32 from (3)]; the sixth line of (9), from the 4 equations related to  $t_{4,2}$  [lines 33-36 from (3)]; the 7th line of (9), from the 4 equations related to  $t_{2,1}$  [lines 21-24 from (3)]; and finally, the 8th line of (9), from the 4 equations related to  $t_{3,4}$  [lines 17-20 from (3)]. After this step the parameter  $p$  is expressed from the 37th row of (3), i.e. the equation for  $\epsilon_0$ .

At this moment 33 equations from (3) are satisfied, all unknown variables (i.e. all block operator parameters and  $p$ ) have (stochastic) values, and only 9 equations remained [lines 25-28, and lines 38-42 from (3)], namely those written for the  $t_{2,3}$  group of 4 relations and the equations for  $\epsilon_1, \epsilon_2, U_1, U_2, U_0$ , which have to be checked. The results of the checking is introduced in a cost function  $K = \sum_{k=1,9} |L_k - R_k|$ , where  $L_k, (R_k)$  represents the left (right) side of the checked  $k = 1, 2, \dots, 9$  equations. The stochastic generation of the parameters from (8) is driven by the minimization of the cost function  $K$ .

## 6 Conclusion

The exact transformation in positive semidefinite form of a Hubbard type of Hamiltonian describing in the present case a non-integrable fermionic itinerant chain with quadrilateral cell is presented in details. The transformation has the peculiarity that both the kinetic and interaction parts of the Hamiltonian are provided by the same positive semidefinite operators. These last are constructed from block operators which contain besides linear fermionic operator contributions, also nonlinear contributions written from three fermionic operators. The transformation holds when the matching equations, a coupled non-linear algebraic system of equations are satisfied, whose solving technique is also indicated. We note that also exact diagonalization steps have been used for checking different results. The procedure works in principle for Hubbard type of Hamiltonian describing other systems as well independent on dimensionality.

We underline, that such transformations are important since Hamiltonians written in positive semidefinite form are objectives of a powerful technique which allows the deduction of exact results for non-integrable quantum mechanical many-body systems.

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#### References:

- [1] D. C. Mattis, *The Many-body Problem: An Encyclopedia of Exactly Solved Models in One Dimension*, World Scientific, Singapore–New Jersey–London–Hong Kong 1993
- [2] V. E. Korepin and F.H.L. Essler, *Advanced Series in Mathematical Physics Vol. 18: Exactly Solvable Models of Strongly Correlated Electrons*, World Scientific, Singapore–New Jersey–London–Hong Kong 1994
- [3] A. Das, *World Scientific Lecture Notes in Physics Vol. 30: Integrable Models*, World Scientific, Singapore–New Jersey–London–Hong Kong 1989
- [4] G. M. D’Ariano, A. Montorsi and M. G. Resetti, *Series on Advances in Statistical Mechanics Vol. 1: Integrable Systems in Statistical Mechanics*, World Scientific, Singapore 1985
- [5] Z. Gulacsi and M. Gulacsi, Exact Solution for a Chainlike Cluster Growth Model, *Phys. Rev. Lett.* 73, 1994, pp. 3239–3242.
- [6] Z. Gulacsi, Exact Ground States of Correlated Electrons on Pentagon Chains, *Int. Jour. Mod. Phys. B* 27, 2013, pp. 1330009-1 – 1330009-64.
- [7] Z. Gulacsi, Exact Results for Non-integrable Systems, *Jour. of Phys. Conf. Ser.* 410, 2013, pp. 012011-1 – 012011-5.
- [8] D. J. Klein, Exact Ground States for a Class of Antiferromagnetic-Heisenberg Models with Short-Range Interactions, *Jour. of Phys. A: Math. Gen.* A15, 1982, pp. 661–671.
- [9] U. Brandt and A. Gieseckus, Hubbard and Anderson Models on Perovskitelike lattices: Exactly Solvable Cases, *Phys. Rev. Lett.* 68, 1992, pp. 2648–2651.
- [10] R. Strack, Exact Ground-State Energy of the Periodic Anderson Model in  $D=1$  and Extended Emery Models in  $D=1,2$  for Special Parameter Values, *Phys. Rev. Lett.* 70, 1993, pp. 833–836.
- [11] H. Tasaki, Exact Resonating-Valence-Bond Ground State and Possibility of Superconductivity in Repulsive Hubbard Models, *Phys. Rev. Lett.* 70, 1993, pp. 3303–3306.
- [12] R. Strack and D. Vollhardt, Hubbard Model with Nearest-Neighbor and Bond-Charge Interaction: Exact Ground-State Solution in a Wide Range of Parameters, *Phys. Rev. Lett.* 70, 1993, pp. 2637–2640.
- [13] P. Gurin and Z. Gulacsi, Exact Solutions for the Periodic Anderson Model in Two Dimensions: A Non-Fermi Liquid State in the Normal Phase, *Phys. Rev.* B64, 2001, pp. 045118-1 – 045118-20.
- [14] Z. Gulacsi and D. Vollhardt, Exact Insulating and Conducting Ground States of a Periodic Anderson Model in Three Dimensions, *Phys. Rev. Lett.* 91, 2003, pp. 186401-1 – 186401-4.
- [15] Z. Gulacsi, Exact Multi-Electronic Electron-Concentration Dependent Ground States for Disordered Two-Dimensional Two-Band Systems in Presence of Disordered Hoppings and Finite On-site Random Interactions, *Phys. Rev.* B69, 2004, pp. 054204-1 – 054204-10.
- [16] Z. Gulacsi, Delocalization Effect of the Hubbard Repulsion in Exact Terms and Two Dimensions, *Phys. Rev.* B77, 2008, pp. 245113-1 – 245113-10.
- [17] Z. Gulacsi and M. Gulacsi, Exact Stripe, Checkerboard, and Droplet Ground States in Two Dimensions, *Phys. Rev.* B73, 2006, pp. 014524-1 – 014524-6.
- [18] Z. Gulacsi, Interaction-Created Effective Flat Bands in Conducting Polymers, *Eur. Phys. Jour.* B87, 2014, pp. 143-1 – 143-10.
- [19] Z. Gulacsi, A. Kampf and D. Vollhardt, Exact Many-Electron Ground States on the Diamond Hubbard Chain, *Phys. Rev. Lett.* 99, 2007, pp. 026404-1 – 026404-4.
- [20] Z. Gulacsi, A. Kampf and D. Vollhardt, Exact Many-Electron Ground States on Diamond and Triangle Hubbard Chains, *Progr. Theor. Phys. Suppl.* 176, 2008, pp.1–21.
- [21] Z. Gulacsi, A. Kampf and D. Vollhardt, Route to Ferromagnetism in Organic Polymers, *Phys. Rev. Lett.* 105, 2010, pp. 266403-1 – 266403-4.
- [22] A. Messiah, *Quantum Mechanics*, Dover Publications Inc., Mineola – New York 1999.